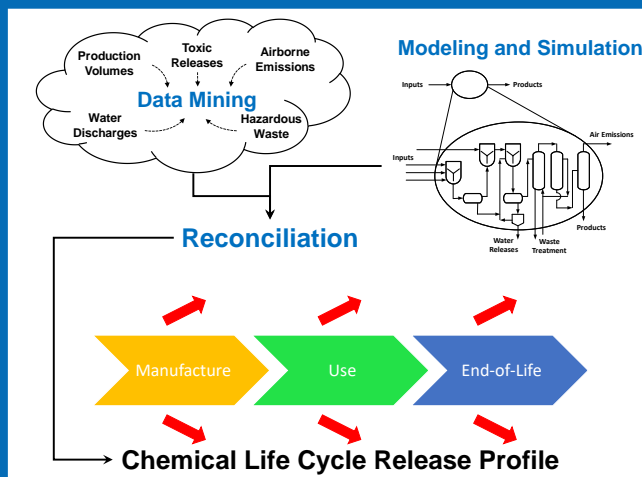


Life Cycle Inventory Modeling at EPA: From Workflows to StEWI

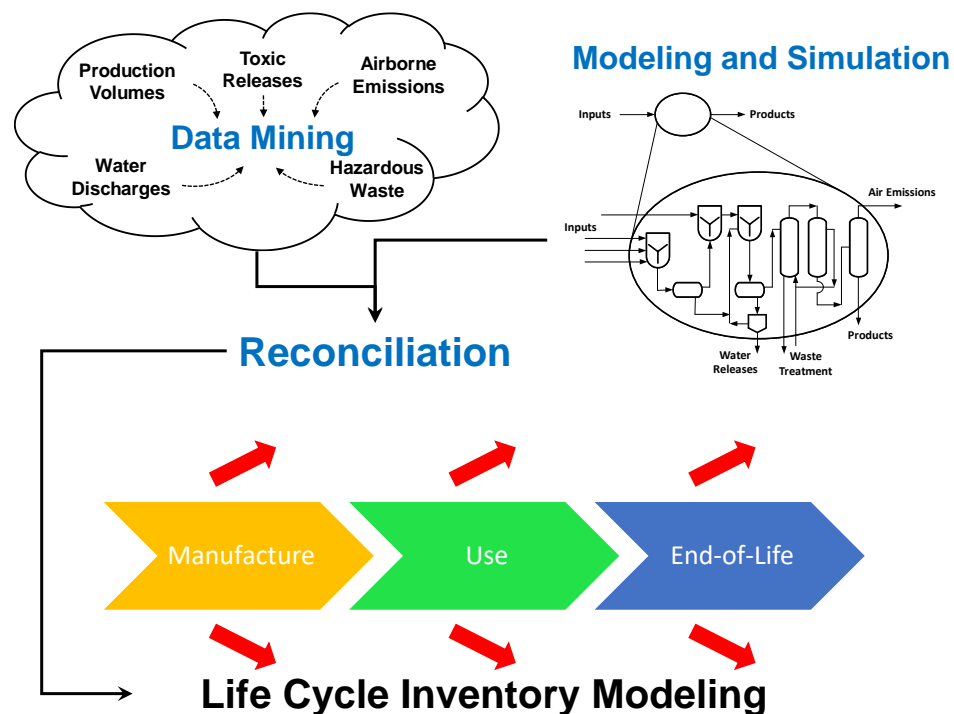
David E. Meyer, William Barret, Michael Gonzalez, Wesley Ingwersen, Gerardo Ruiz-Mercado, Raymond Smith



eLCAd – March 31, 2021

Overview

- Inventory Modeling Challenges at EPA
- Building a Toolbox with Secondary Data
 - Data Mining
 - Simulation
 - Automation
- Takeaways



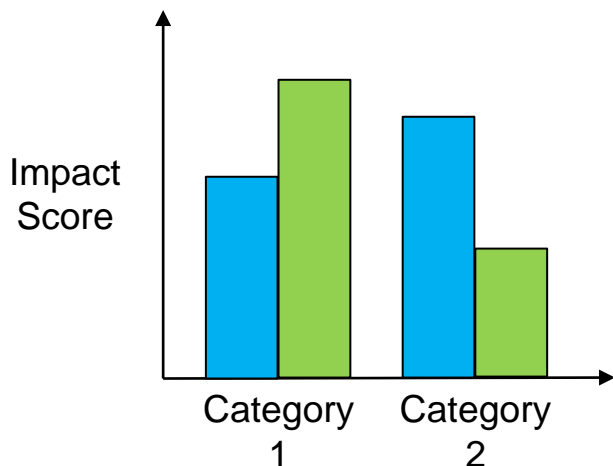


Disclaimer

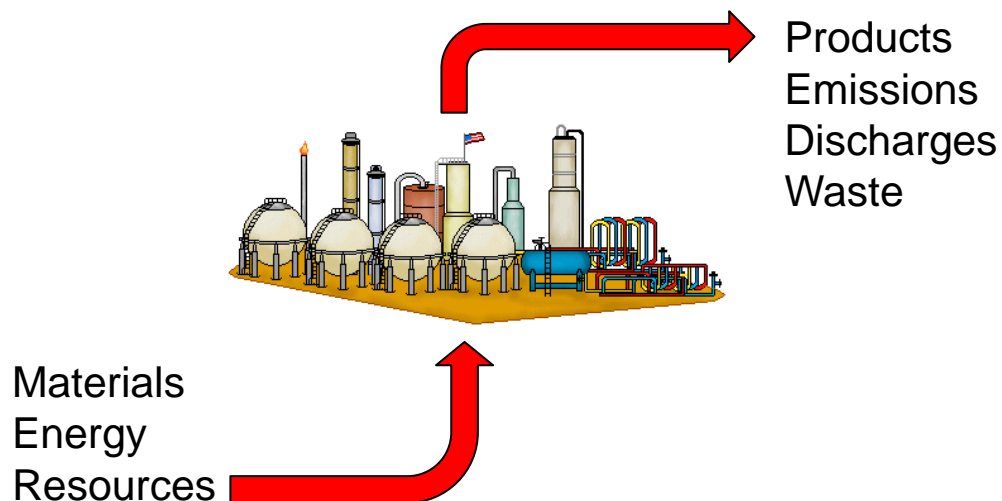
The views expressed in this presentation are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

The Origin Story: LCA and Inventory Modeling

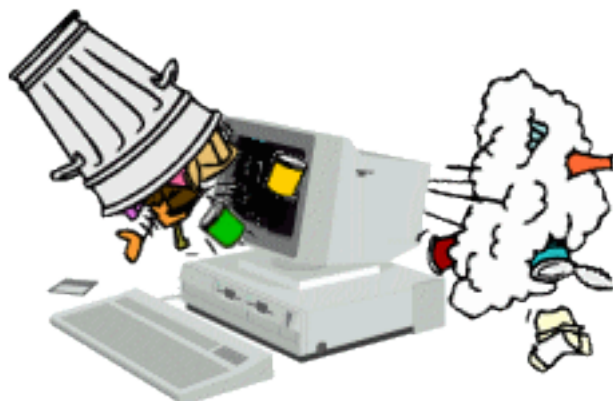
You can't get this...



... without this!



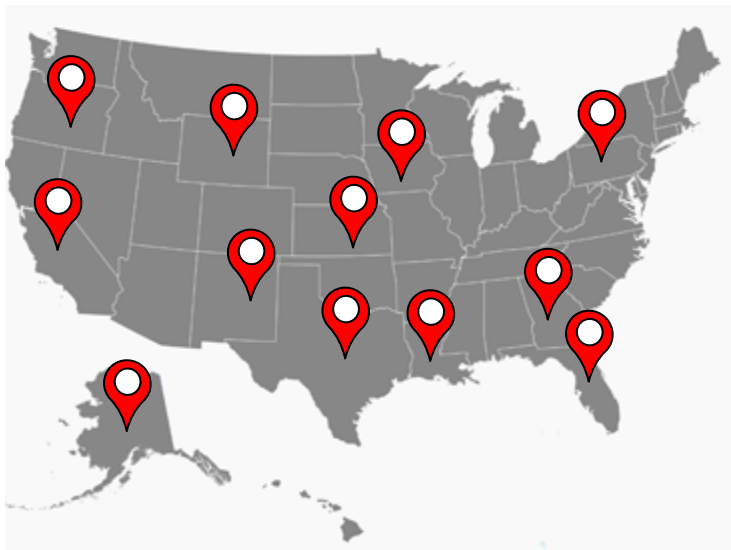
- The success of an LCA is highly dependent on the Life Cycle Inventory (LCI).**



Garbage In = Garbage Out

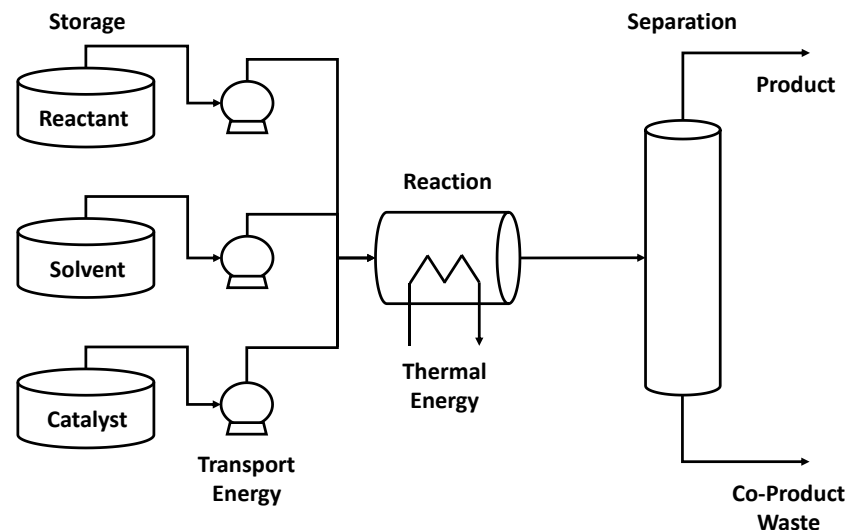
LCI at EPA: Inventories of Scale

Sector



Vs.

Process

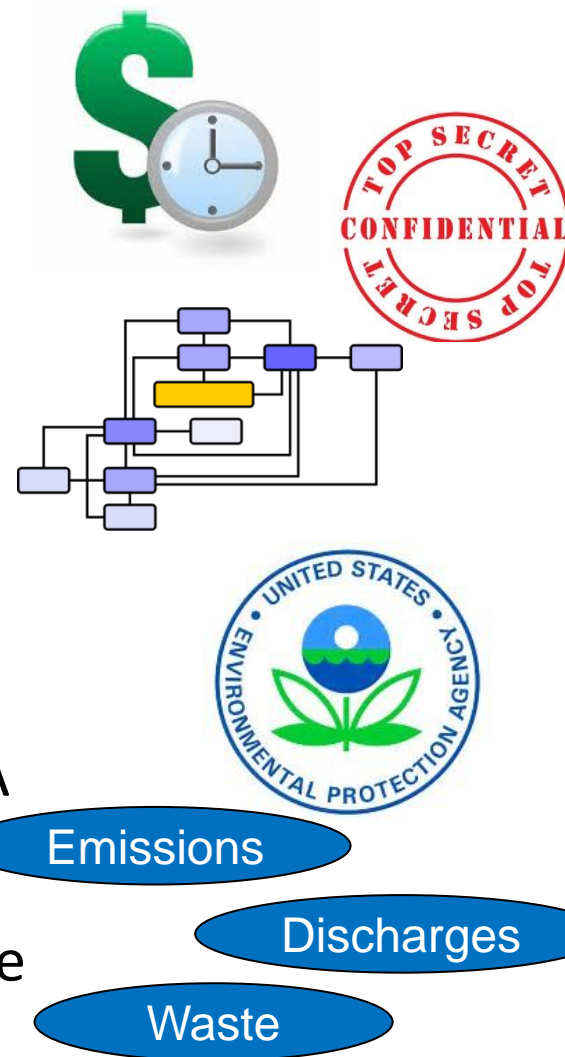


- Develop LCI by NAICS classification
- **Uses:** Environmentally Extended Input-Output LCA (EEIO-LCA)
- **Challenges:** millions of data points; multi-NAICS facilities; aggregate products and functional unit

- Develop LCI for a specific chemical
- **Uses:** Exposure modeling; Process LCA
- **Challenges:** multi-product facilities; CBI data; unknown production volumes

Rapid and Reliable LCI: the Issues

- Field data = the best = resource intensive
- Most chemical process data for the US are proprietary
- Cradle-to-gate chemical LCI may involve hundreds of processes
- EPA has a trove of data that could be useful for LCA
- EPA is both a consumer and provider of LCA data
- EPA data needs to be reproducible, reusable and publically available



Building a Comprehensive Toolbox: Data Mining (Top Down)

- Multiple publicly available EPA data sources:

Database	Production Volume	Air Emissions	Water Discharges	Hazardous Waste
Chemical Data Reporting Tool (CDR)	X			
Discharge Monitoring Report (DMR)			X	
Greenhouse Gas Reporting Tool (eGGRT)		X		
National Emissions Inventory (NEI)		X		
RCRAInfo				X
Toxics Release Inventory (TRI)		X	X	X

DOI: [10.1021/acs.est.6b02160](https://doi.org/10.1021/acs.est.6b02160)
Environ. Sci. Technol. 2016, 50,
9013–9025



Policy Analysis
pubs.acs.org/est

Mining Available Data from the United States Environmental Protection Agency to Support Rapid Life Cycle Inventory Modeling of Chemical Manufacturing

Sarah A. Cashman,[†] David E. Meyer,^{*‡} Ashley N. Edelen,^{§,||} Wesley W. Ingwersen,[‡] John P. Abraham,[‡] William M. Barrett,[‡] Michael A. Gonzalez,[‡] Paul M. Randall,[‡] Gerardo Ruiz-Mercado,[‡] and Raymond L. Smith[‡]

Method: The Nuts and Bolts

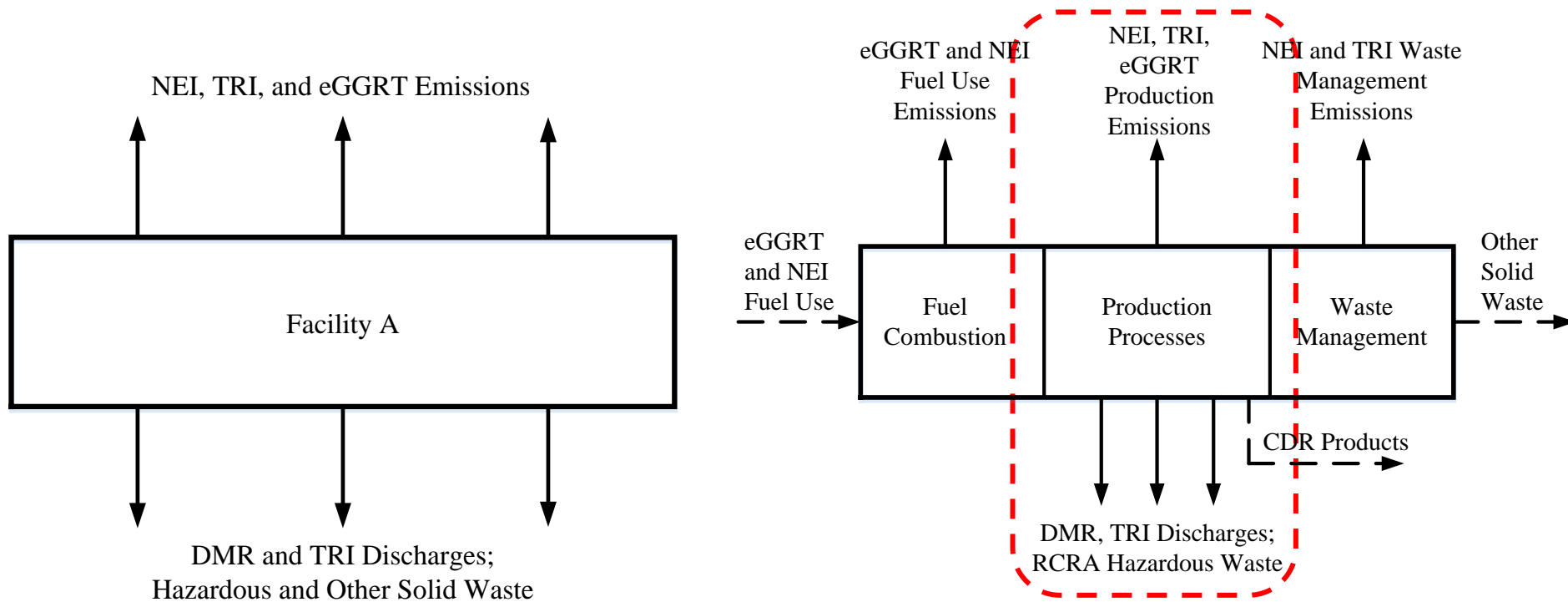
- Create a weighted-average chemical manufacturing unit process

$$\overline{EF}_{Pollutant\ X}^{PD} = \frac{\sum_i^N (EF_{Pollutant\ X, Facility\ i} \times PV_{PD, Facility\ i})}{\sum_i^N PV_{PD, Facility\ i}}$$

Where:

- $\overline{EF}_{Pollutant\ X}^{PD}$ is the weighted average emission factor, specific to pollutant X and, in this example, the production of the chemical product (kg/kg)
- $EF_{Pollutant\ X, Facility\ i}$ is an emission factor for pollutant X at a specific facility (a pollutant emission normalized by total chemical production, kg/kg)
- $PV_{PD, Facility\ i}$ is the production volume of the chemical product at a specific facility (kg)
- Subscript *Pollutant X* refers to a unique pollutant-media combination (e.g., CO₂ emissions to air, ammonia emissions to water)
- Subscript *Facility i* refers to a specific facility (e.g., Facility A)
- *N* is the total number of all facilities
- *PD* refers to the chemical product of interest



Facility vs. Activity Modeling



- For detailed chemical assessments, need release of chemical by activity.
- Ancillary activities (energy, waste treatment) are modeled separately to allow flexibility.

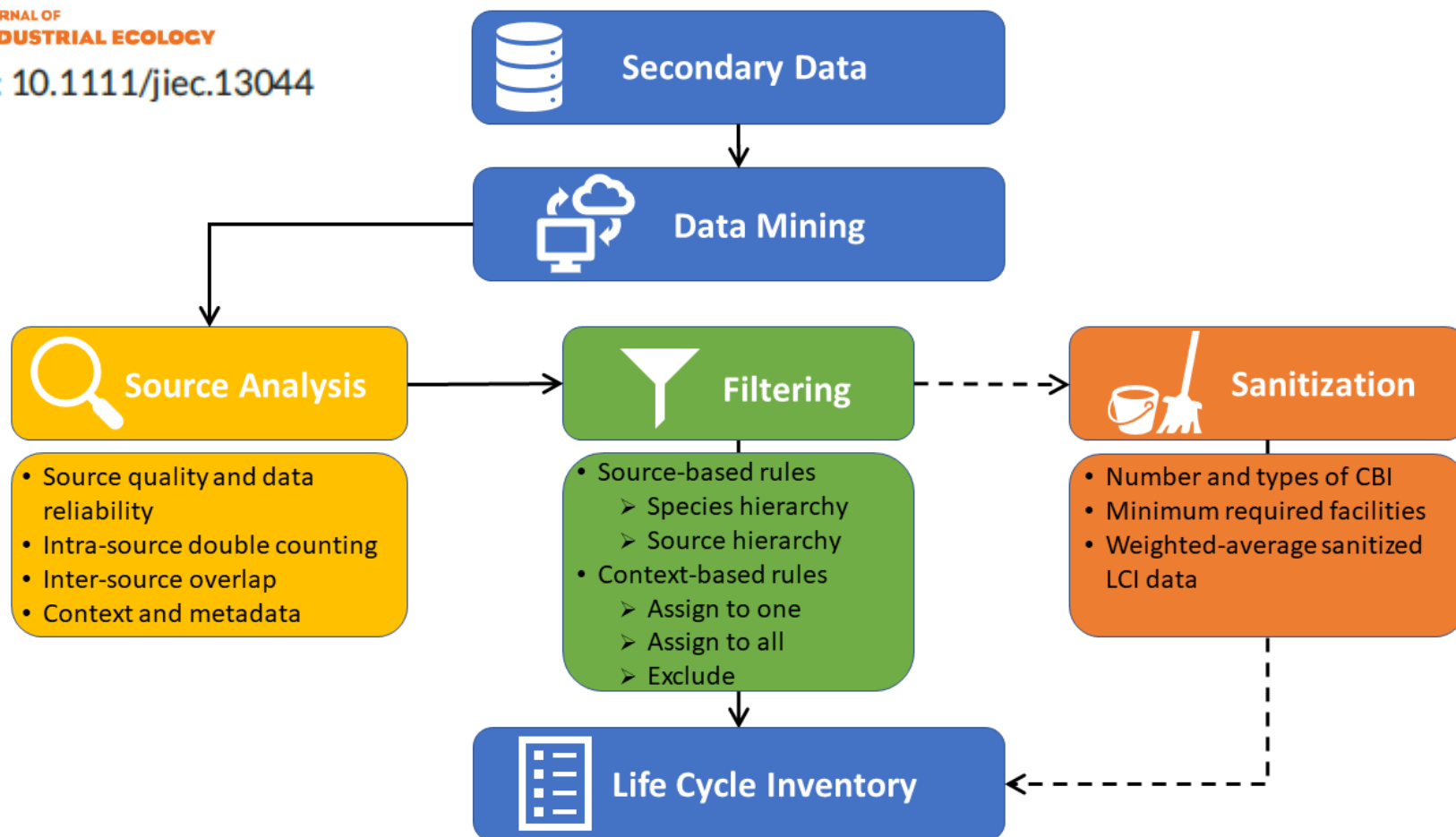
Integrating Metadata to Improve Data Model Quality

Improving the reliability of chemical manufacturing life cycle
inventory constructed using secondary data

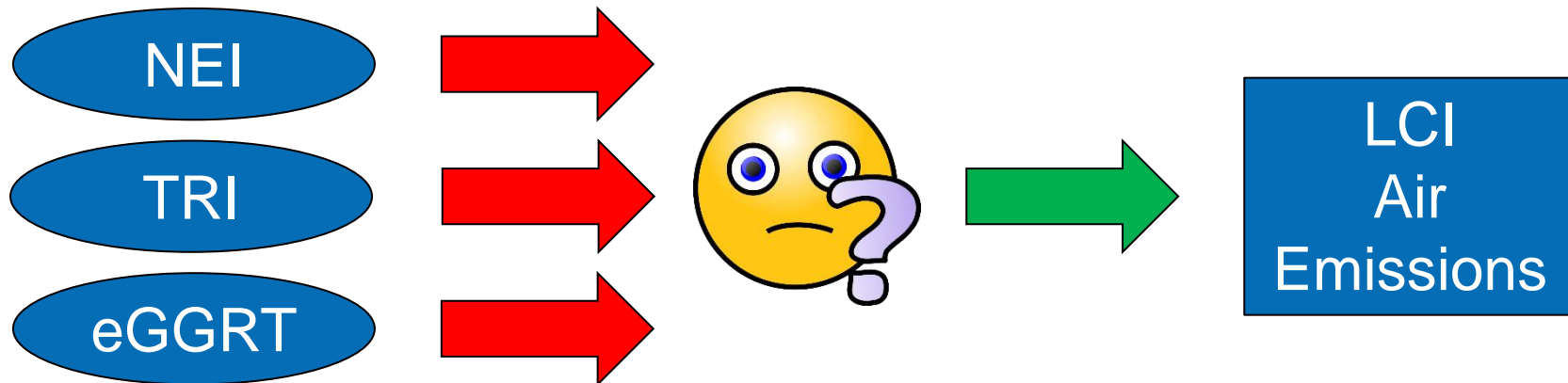
David E. Meyer¹  | Sarah Cashman²  | Anthony Gaglione²

 JOURNAL OF
INDUSTRIAL ECOLOGY

DOI: 10.1111/jiec.13044



Resolving Inter-Database Overlap



- ***NEI over TRI*** (greatest overlap between these databases)
 - Overlap related to HAPS
 - Facilities more accountable for toxics under TRI, but reporting lacks process specificity
 - Need to use NEI over TRI to employ process-level allocation
 - If not conducting process-level allocation, could select database based on flow reliability score
- ***eGGRT over NEI*** for GHG overlap

Examples of Handling Intra-Database Speciation

impact characterization, speciated emissions are always preferred because they are more compatible with characterization factors. Note: For

Data Source	Chemical Group	Rule	Adjustment
NEI	Particulate Matter	Select primary PM10 and PM2.5	$PM10_{Adjusted} = PM10_{PRI} - PM2.5_{PRI}$
NEI	Volatile Organic Compounds	Select individual species over VOC group totals	$VOC_{Adjusted} = VOC_{Reported} - \sum Species$
NEI	Polycyclic Organic Matter	Facilities can report by either species or group, but not both	None
DMR	Chemical and Biological Oxygen Demand	Facilities can report both groups	Prioritize COD for chemical sector and filter out BOD

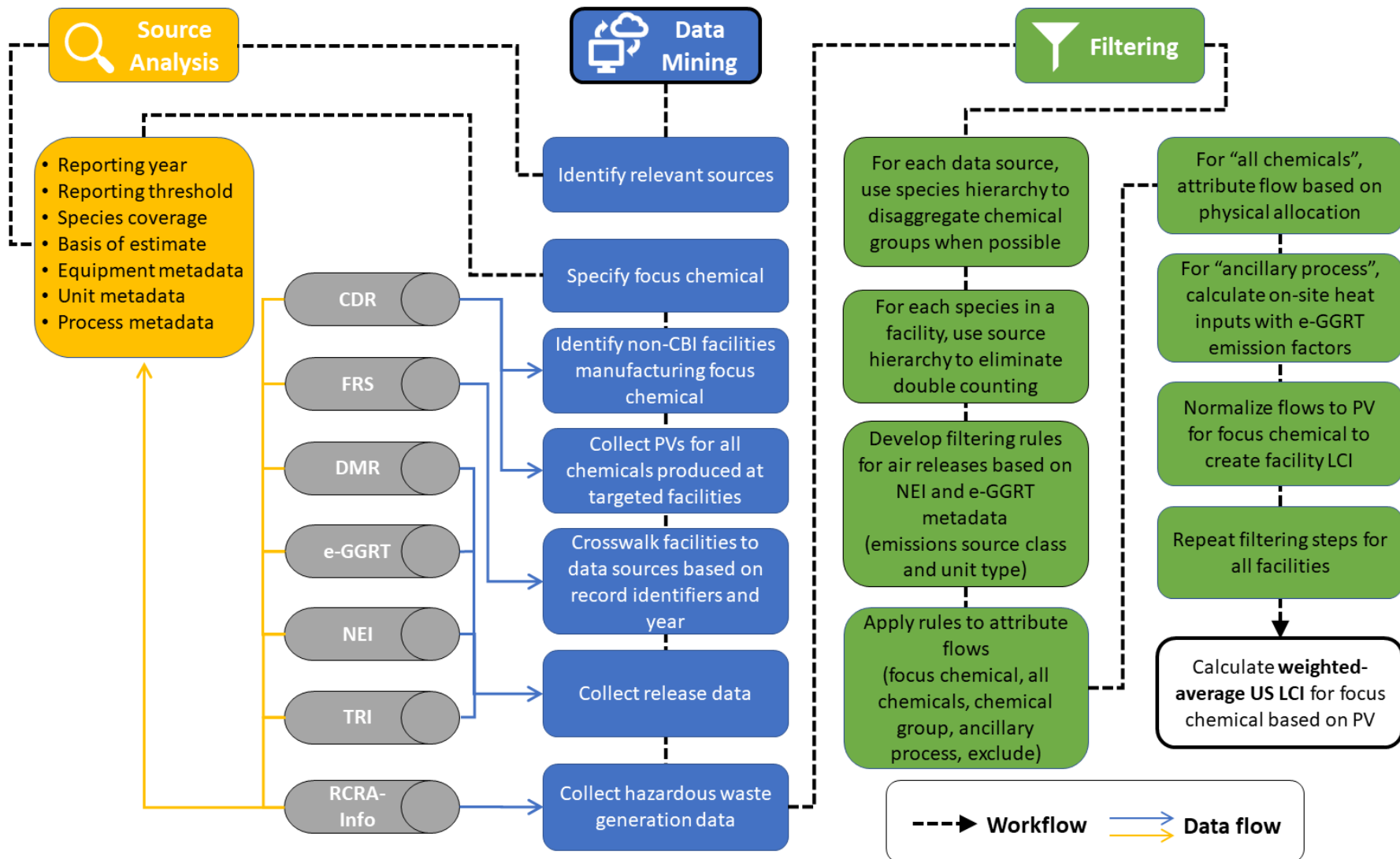
Assessing Data Quality

- **Flow reliability** based on reporting method

Code	Description	Type	Reliability
1	Continuous monitoring system	Verified measurement	1
2	Engineering Judgement	Undocumented estimate	5
3	Material Balance	Undocumented estimate	5
4	Stack Test	Verified measurement	1
5	USEPA Speciation Profile	Verified calculation	2
7	Manufacturer Specification	Undocumented estimate	5
8	US EPA Emission Factor (no control efficiency used)	Verified calculation	2
9	S/L/T Emission Factor (no control efficiency used)	Verified calculation	2
10	Site-specific emission factor (no control efficiency used)	Verified calculation	2
28	USEPA Emission Factor (pre-control) plus Control Efficiency	Verified calculation	2

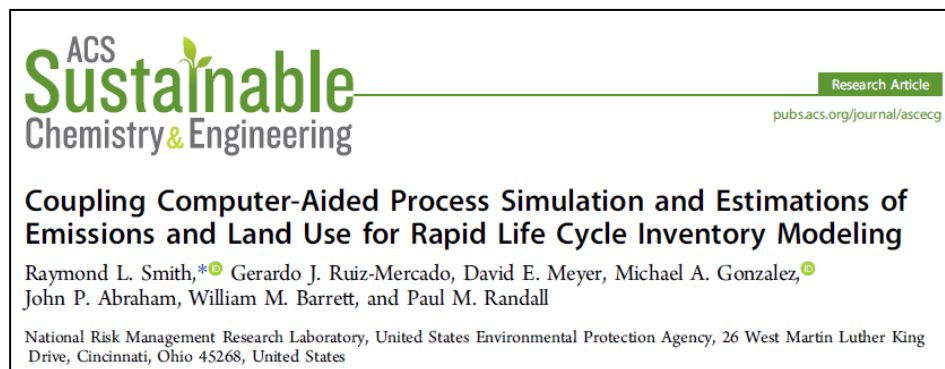
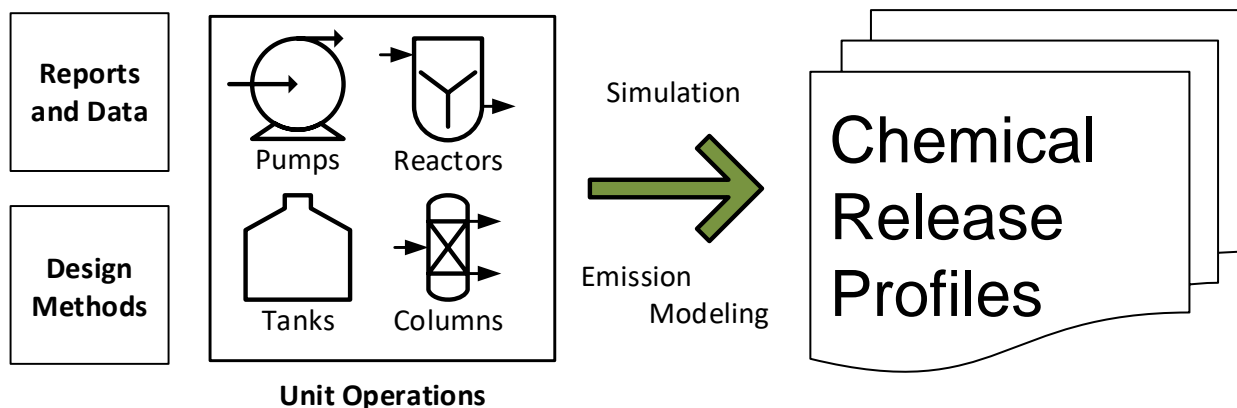
- **Temporal correlation** based on reporting year
- **Geographical correlation** = 1 as method only covers U.S. facilities (assuming level of resolution is national)
- **Technological correlation** depends on the ability to determine the technology used by a facility (based on NEI and GHGRP metadata) and the coverage of total U.S. production
- **Sampling methods correlation** depends on the percentage of total U.S. production captured by CDR

A New and Improved Workflow



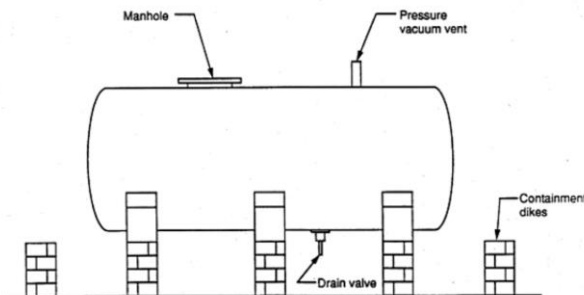
Building a Comprehensive Toolbox: Process Simulation (Bottom Up)

Advantages: activity specific; potential for improved release estimations; storage, vent, and fugitive emissions included

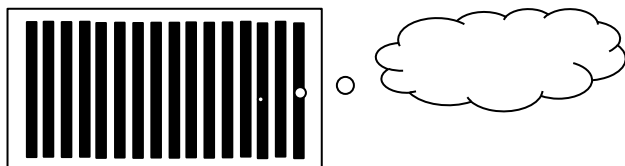


Challenges: knowledge of engineering design; need for chemical synthesis details; uncontrolled emissions

Storage



Venting



$$E_i = \frac{F x_i \gamma_i P_i^{sat}}{RT} S_i (MW_i)$$

U.S. EPA (1994) *Hdbk Control Techniques for Fugitive VOC Emissions*; Hatfield, J.A. (2004) *Env. Prog.*, 23, 45

Realistic Simulation: Uncontrolled Emissions

$$\text{Working losses: } L_W = \frac{\dot{V}}{22.4} \left(\frac{273.15}{T} \right) \left(\frac{P_i^{sat}}{760} \right) (MW) K_N K_P$$

$$\text{Breathing losses: } L_B = 16.3 V_V \left(\frac{273.15}{T} \right) \left(\frac{P_i^{sat}}{760} \right) (MW) \left(\frac{T_R}{T} \right)$$

U.S. EPA (2016) *AP-42*, Ch. 7; Peress, J. (2001) *CEP*, Aug. 44-45

Fugitive Emissions

Equipment Type	Service	Emission Factor (kg/h/source)
Pumps	Light liquid	0.0199
	Heavy liquid	0.00862
Compressors	Gas	0.228
Valves	Gas	0.00597
	Light liquid	0.00403
	Heavy liquid	0.00023
Connectors (e.g., flanges)	All	0.00183
Open-ended lines	All	0.0017
Sampling connections	All	0.0150
Pressure relief valves	Gas	0.104

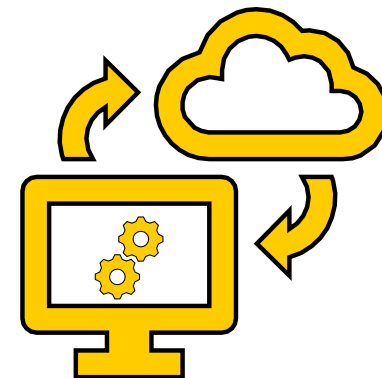
Synthetic Org. Chem. Mfg. Ind., U.S. EPA (1995)
Protocol for Equipment Leak Emission Estimates

Simulated Emissions During Acetic Acid Manufacturing

LCI Outputs	Simulation			Simulation and Emission Models		
(kg/kg Acetic Acid Product)	Fugitive	Storage	Vents	Fugitive	Storage	Vents
Carbon Monoxide			2.18E-02	1.77E-05		4.36E-02
Carbon Dioxide			1.72E-03	7.94E-07		3.50E-03
Methane			6.37E-04	2.90E-07		1.27E-03
Methanol			1.90E-03	1.52E-05	1.85E-04	1.90E-03
Acetic Acid				3.17E-05	5.07E-05	7.15E-04
Methyl Iodide			6.92E-03	2.78E-05	2.29E-05	8.13E-03
Hydrogen Iodide			2.02E-03	1.07E-06		2.09E-03
Methyl Acetate			1.33E-03	1.10E-05		2.23E-03
Water			5.18E-07	2.64E-05		6.93E-06
Propionic Acid				1.83E-08		3.12E-07

- Including uncontrolled emissions introduces additional emission sources for impact assessment.

Automated Inventory Modeling: StEWI



- **Standardized Emissions and Waste Inventories**
(<https://github.com/USEPA/standardizedinventories>)
 - Collection of **Python modules** that **process USEPA emission and waste generation data** into standard tabular formats.
 - Standard outputs can be (1) aggregated or filtered based on given criteria; and (2) combined based on common facility and flows across the inventories

USEPA Inventories Covered By Data Reporting Year (current version)

Source	2011	2012	2013	2014	2015	2016	2017	2018
Toxic Release Inventory	x	x	x	x	x	x	x	x
RCRA Biennial Report	x		x		x		x	
National Emissions Inventory*	x			x		x	x	
Emissions & Generation Resource Integrated Database				x		x		x

*Only point sources included at this time from NEI

What StEWI Can Give Us

- Multiple output formats

Flow-By-Facility	Total annual release or waste flow of a single compound by facility
Flow-By-SCC (activity info)	Total annual release or waste flow of a single compound by facility by source classification code (SCC)
Facility (List)	List of unique facilities in a given inventory and given year
Flow (List)	Each row represents a unique flow (substance or waste) in a given inventory and given year (“Flow List”)

- Combined output – StEWICombo

➤ optionally remove overlaps based on user preferences

Flow-By-Facility Combined	Analogous to Flow-By-Facility, with chemical and facility matches added in
------------------------------	--

Conclusions

- Life cycle inventory modeling using secondary data can be **tailored to fit assessment needs** by using a variety of approaches.
- **Data mining** is a suitable approach for existing chemicals. The **quality** of the release profile is **dependent on production coverage and the availability of metadata** to properly allocate releases to activities.
- **Modeling and simulation** can provide release estimates for both existing and new chemicals. The **quality** of the estimates is **enhanced by including uncontrolled and fugitive emissions**.
- **Automation and data harmonization** will support more **rapid inventory modeling**.

“Ambient informatics is a state in which information is freely available at the point in space and time someone requires it, generally to support a specific decision.”

- Adam Greenfield - Everyware

Feel Free to Discuss!

"A single conversation across the table with a wise person is worth a month's study of books"

- Chinese Proverb

Data Mining Examples

- Objective:** Develop U.S. national-average profiles for the production of Acetic Acid and Cumene (or (Propan-2-yl)benzene)

	Acetic Acid	Cumene
Total # of Facilities	25	10
CBI Facilities	17	2
Public Facilities	8	8
% of Total Production Volume	1.17%	80.75%

Low coverage without CBI facilities

of Reporting Facilities (Public CDR Only) for 2011 Databases

	<u>NEI</u>	<u>TRI</u>	<u>DMR</u>	<u>RCRAinfo</u>
Acetic Acid	7	8	4	3
Cumene	8	8	7	8

- Working with multiple EPA databases can be challenging because of variations in reporting thresholds and requirements.

Learning from the Metadata

Filter using additional information about an emission:

SCC codes

process and unit descriptions

NEI Unit Description	NEI Unit Type Description	NEI Unit Type Group	NEI Process Description	Action
T007, 1-7-TK-7 Cumene Storage Tank	Storage Tank	Evaporative Sources	CUMENE BL TANK 7	Allocate 100% to cumene
CT07, 2-603-CT-05 New North area cooling tower	Unclassified	Unclassified	2-603-CT-5, NNA	Allocate across all chemicals
T855, 2-606-TK-855 Gas Oil / Distillate Tank	Storage Tank	Evaporative Sources	DISTILLATE TANK 855 WL	Exclude - unrelated
H042, 1-35-B-03 Cumene Column Reboiler	Process Heater	Fuel Comb. Equipment	1-35-B-3 1 CUMENE COL REB	Exclude - energy process

Source	Substance	Value		Unit	Change	
		Raw	Filtered		%	DQ Score
eGGRT	carbon dioxide	1.40E-02	2.14E-03	kg	-85%	3.43
eGGRT	dinitrogen monoxide	8.01E-08	1.32E-08	kg	-83%	3
eGGRT	methane	7.28E-06	6.95E-06	kg	-5%	3.89
NEI	1,3-Butadiene	0	0	kg	-	2
NEI	2,2,4-Trimethylpentane	0	0	kg	-	2
NEI	Ammonia	1.266E-08	0	kg	-100%	5
NEI	Benzene	3.354E-07	2.34E-05	kg	6889%	2
NEI	Biphenyl	2.223E-10	0	kg	-100%	5
NEI	Carbon Disulfide	7.04E-09	0	kg	-100%	5
NEI	Carbon Monoxide	9.756E-06	0	kg	-100%	2
NEI	Cobalt	3.705E-11	0	kg	-100%	5
NEI	Cumene	1.169E-07	2.50E-05	kg	21319%	2
NEI	Ethyl Benzene	0	0	kg	-	2
NEI	Ethylene Dichloride	5.138E-11	0	kg	-100%	2
NEI	Hexane	0	0	kg	-	2
NEI	Hydrochloric Acid	3.869E-07	0	kg	-100%	5
NEI	Hydrogen Fluoride	5.632E-10	0	kg	-100%	5
NEI	Hydrogen Sulfide	0	0	kg	-	2
NEI	Lead	1.96E-11	0	kg	-100%	2
NEI	Mercury	3.283E-10	0	kg	-100%	5
NEI	Methanol	4.091E-09	0	kg	-100%	5
NEI	Methyl Tert-Butyl Ether	0	0	kg	-	2
NEI	Naphthalene	0	0	kg	-	2
NEI	Nickel	9.856E-10	0	kg	-100%	5
NEI	Nitrogen Oxides	3.489E-06	0	kg	-100%	2
NEI	PAH, total	1.438E-10	0	kg	-100%	5
NEI	PM10 Primary (Filt + Cond)	1.738E-06	1.46E-06	kg	-16%	2
NEI	PM2.5 Primary (Filt + Cond)	1.701E-06	1.44E-06	kg	-16%	2
NEI	Styrene	0	0	kg	-	2
NEI	Sulfur Dioxide	2.81E-06	0	kg	-100%	2
NEI	Toluene	5.072E-08	0	kg	-100%	2
NEI	Volatile Organic Compounds	1.599E-05	3.88E-05	kg	143%	2
NEI	Xylenes (Mixed Isomers)	0	0	kg	-	2

Cumene U.S.-Average Emission Profile

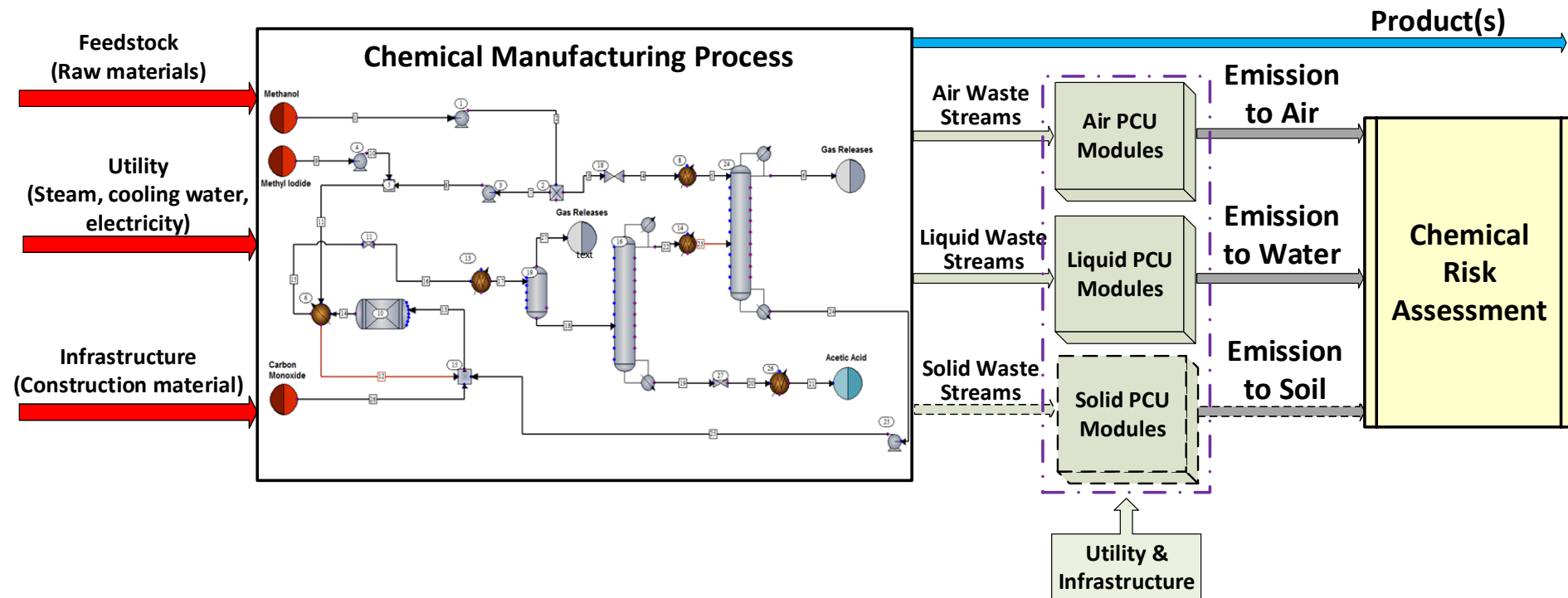
Substance	Value	Unit	Flow Count	DQI Score	Database
1,2,4-TRIMETHYLBENZENE	4.4E-08	kg	5	2.15	TRI
1,3-Butadiene	1.9E-08	kg	5	1.62	NEI
2,2,4-Trimethylpentane	3.9E-08	kg	4	2	NEI
2-Methylnaphthalene	3.5E-13	kg	1	2	NEI
4,4'-ISOPROPYLIDENEDIPHENOL	1.6E-08	kg	2	3.03	TRI
7,12-Dimethylbenz[a]Anthracene	2.3E-13	kg	1	2	NEI
Acenaphthene	1.2E-13	kg	1	2	NEI
Acetaldehyde	1.1E-07	kg	2	2	NEI
Acetamide	2.2E-11	kg	1	2	NEI
Acetonitrile	1.8E-08	kg	1	2	NEI
Acetophenone	1.2E-06	kg	3	2.25	NEI
ALLYL ALCOHOL	2.0E-09	kg	1	1.91	TRI
Ammonia	3.1E-07	kg	6	2.33	TRI NEI
Antimony	1.5E-11	kg	1	2	NEI
ANTIMONY COMPOUNDS	1.5E-11	kg	1	2	TRI
Arsenic	1.0E-11	kg	1	2	NEI
Benzene	5.6E-06	kg	8	2.19	NEI
Benzo[a]Pyrene	0	kg	1	2	NEI
Benzo[g,h,i]Perylene	5.6E-13	kg	4	3.39	TRI NEI
Beryllium	2.3E-13	kg	1	2	NEI
Biphenyl	0	kg	1	5	NEI
Cadmium	3.6E-11	kg	1	2	NEI
Carbon dioxide	2.3E-03	kg	5	2.10	eGGRT
Carbon Disulfide	0	kg	2	2.64	NEI
Carbon Monoxide	1.2E-07	kg	7	1.83	NEI
CARBONYL SULFIDE	0	kg	2	2.64	TRI NEI
Catechol	4.7E-10	kg	1	2	NEI
Chlorine	1.4E-10	kg	3	4.52	NEI TRI
Chloroform	6.1E-10	kg	1	2	NEI
CHLOROMETHANE	7.0E-09	kg	1	5	TRI
Chromium (VI)	5.8E-13	kg	1	2	NEI
Coal Tar	0	kg	1	2	NEI
Cobalt	0	kg	2	5	NEI
COPPER COMPOUNDS	4.3E-11	kg	1	5	TRI

Substance	Value	Unit	Flow Count	DQI Score	Database
CUMENE	1.9E-05	kg	7	2.21	NEI TRI
CUMENE HYDROPEROXIDE	1.3E-08	kg	3	1.31	TRI
Cyanide	0	kg	1	5	NEI
CYCLOHEXANE	6.5E-08	kg	6	1.99	TRI
DICYCLOPENTADIENE	2.4E-09	kg	1	2	TRI
DIETHANOLAMINE	1.8E-08	kg	3	2.00	TRI NEI
Dinitrogen monoxide	8.7E-09	kg	5	1.99	eGGRT
DIOXIN AND DIOXIN-LIKE COMPOUNDS	4.2E-15	kg	3	2.98	TRI
Epichlorohydrin	9.6E-09	kg	1	1.96	NEI
Ethyl Benzene	4.8E-08	kg	7	1.95	NEI
ETHYLENE	3.1E-07	kg	5	2.12	TRI
Ethylene Dichloride	3.1E-12	kg	2	2	NEI
Ethylene Glycol	1.9E-10	kg	2	3.14	NEI TRI
Fluoranthene	1.2E-13	kg	1	2.00	NEI
Formaldehyde	1.3E-09	kg	2	2	NEI
FORMIC ACID	4.1E-11	kg	1	4.958	TRI
GLYCIDOL	0	kg	1	3.50	TRI
Glycol Ethers	9.4E-10	kg	1	2	NEI
Hexane	8.5E-08	kg	6	2.009	NEI
Hydrochloric Acid	4.2E-09	kg	4	3.744	NEI TRI
Hydrogen Cyanide	6.5E-08	kg	2	1.303	NEI
HYDROGEN FLUORIDE	4.7E-12	kg	3	4.084	NEI
Hydrogen Sulfide	0	kg	1	2.00	NEI
ISOPRENE	1.4E-08	kg	1	3.89	TRI
Lead	2.9E-11	kg	4	4.32	TRI NEI
Manganese	3.1E-10	kg	1	2	NEI
Mercury	1.6E-10	kg	5	2.305	NEI TRI
Methane	2.4E-06	kg	5	2.151	eGGRT
METHANOL	2.3E-08	kg	5	2.51	NEI TRI
Methyl Isobutyl Ketone	4.0E-09	kg	1	2.162	NEI
Methyl Tert-Butyl Ether	7.3E-10	kg	3	2.00	NEI
Methylene Chloride	1.2E-12	kg	1	2	NEI
MOLYBDENUM TRIOXIDE	5.7E-11	kg	2	5	TRI
M-XYLENE	6.9E-10	kg	1	5	TRI

Substance	Value	Unit	Flow Count	DQI Score	Database
Naphthalene	1.2E-08	kg	5	2.00	NEI
Nickel	2.5E-10	kg	3	4.08	NEI
Nitrogen Oxides	6.8E-07	kg	7	1.91	NEI
O-XYLENE	2.8E-10	kg	1	1.75	TRI
Phenanthrene	3.5E-13	kg	1	2	NEI
Phenol	2.4E-07	kg	5	2.66	NEI TRI
Phosphorus	2.1E-11	kg	1	2	NEI
PM10 Primary (Filt + Cond)	1.7E-06	kg	8	2.7887	NEI
PM2.5 Primary (Filt + Cond)	1.4E-06	kg	8	2.5435	NEI
POLYCYCLIC AROMATIC COMPOUNDS	1.7E-09	kg	5	3.2116	TRI NEI
Propionaldehyde	0	kg	1	2	NEI
PROPYLENE	6.2E-06	kg	7	2.1027	TRI
Pyrene	1.2E-11	kg	1	2.00	NEI
Selenium	1.2E-11	kg	1	2.00	NEI
Styrene	9.4E-10	kg	3	2	NEI
Sulfur Dioxide	2.7E-07	kg	7	2.25	NEI
SULFURIC ACID	1.9E-07	kg	2	1.3347	TRI
TERT-BUTYL ALCOHOL	0	kg	1	5.00	TRI
TETRACHLOROETHYLENE	0	kg	3	5.00	TRI NEI
Toluene	1.1E-06	kg	7	2.00	TRI NEI
Vinyl Acetate	1.2E-12	kg	1	2	NEI
Volatile Organic Compounds	5.3E-05	kg	8	2.14	NEI
Xylenes (Mixed Isomers)	8.3E-08	kg	7	2.00	NEI
ZINC COMPOUNDS	1.4E-09	kg	1	5	TRI

**92 substances reported
for the 8 facilities.
26 substances reported
by >4 facilities.**

Abatement Technology Modeling



- **Pollution Control Unit (PCU) Modules** include pollution control technologies for air, liquid and solid wastes
- Controlled air, water, and solid emissions from single chemical modeling (**PCU Modules**) provide better estimates for **chemical RA**

Abatement Technology Modeling: Acetic Acid Manufacturing Example

LCI Input	Units*	Simulation	Simulation with PCUs	Percentage Change*
Steam	kg/kg AA	7.7900E-01	4.9458E-01	-37%
Natural Gas	scm/kg AA	0.0000E+00	2.3408E-02	∞
Purge Gas	scm/kg AA	0.0000E+00	1.2423E-03	∞
Solvent (Water)	kg/kg AA	0.0000E+00	2.4749E+00	∞
Electricity	kW/kg AA	5.5980E-03	5.7381E-03	3%
Material	kg/(kg AA per year)	2.0346E-06	1.6940E-05	733%
Footprint	m ² /(kg AA per year)	1.0230E-04	1.0472E-04	2%
LCI Output				
Carbon Monoxide	kg/kg AA	4.3848E-02	8.7306E-04	-98%
Carbon Dioxide	kg/kg AA	5.4548E-04	1.3619E-01	24868%
Methane	kg/kg AA	1.9675E-04	1.0879E-09	-100%
Methanol	kg/kg AA	3.0957E-05	0.0000E+00	-100%
Acetic Acid	kg/kg AA	2.60E-02	0.0000E+00	-100%
Hydrogen Iodide	kg/kg AA	1.8368E-03	0.0000E+00	-100%

Results correspond to waste streams associated with Acetic Acid (AA) manufacturing process example simulated in CHEMCAD, in which “-” represents decrease (in percentage) while “∞” represents division by zero in calculation of percentages (for cases without corresponding inlet stream)